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PREFACE

The Euro-Asian Symposium “Trends in Magnetism” (EASTMAG 2001), organized by the Institute of Metal Physics, Russian Academy of Sciences, was held in the Ural Cultural Center, Ekaterinburg, Russia, from February 27 to March 2, 2001, under the motto “At the Border of Two Continents, at the Boundary of Centuries”.

The purpose of the symposium was to provide an opportunity for scientists from all over the world to meet at the border of Europe and Asia to discuss recent advances in the study of the physics of magnetic materials. The EASTMAG symposia are aimed at continuing and developing the best traditions of the former All-Union Conferences on Magnetism that were organized previously in the former Soviet Union. EASTMAG 2001 was devoted to the memory of academician S.V. Vonsovsky, who made a great contribution to magnetism, and the development of science in Russia. Two hundred fifty participants from 15 countries took part.

Three supplementary issues of volumes 91, 92, and 93 of *The Physics of Metals and Metallography* contain the papers presented at the symposium and accepted for publication through a review process determined by *The Physics of Metals and Metallography.* Supplementary issues nos. 1 of vols. 91–93 consist of nine chapters devoted to the physics of new magnetic materials: multilayers and films, nanocrystalline and amorphous materials, manganites, hard magnetic materials, domain structures and domain walls, resonances, excitations, waves, model systems and computations, novel scientific instrumentation, and finally, magnetic alloys and compounds.

On behalf of the organizing committee, I would like to express my sincere gratitude to all the participants of the symposium for their excellent contributions and to the authors who presented papers for the proceedings. I hope that the proceedings provide valuable information on the physics of magnetic phenomena and technology of magnetic materials.

March 2001
Vladimir Ustinov
EASTMAG 2001 Chairman

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Electronic Structure and Magnetic Mechanism of Pairing in HTSC Transition Metal Oxides

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Abstract—Starting from the multiband *p–d* model of strongly correlated electrons, we derive the effective Hamiltonian in the form of the generalized singlet–triplet *t–t'–J* model which transforms to the usual *t–t'–J* model in the low-energy limit. Both *n*- and *p*-type copper oxides are considered in the mean field approximation for Gorkov type Green functions in the *X*-operator representation. Different signs of the t'/t ratio result in different normal state properties and T_c values conserving the $d_{x^2-y^2}$ gap symmetry both for *n*- and *p*-oxides. Comparison with ruthenates and the coexistence of superconductivity and magnetism in $RuSr_2GdCu_2O_8$ are studied in the extended *t–J–I* model with ferromagnetic coupling between Ru ions.

INTRODUCTION

Currently, there is no widely accepted theory for the electronic structure of the undoped antiferromagnetic insulator, its concentration evolution with doping to the metal state, and for the pairing mechanism in cuprates of *p*- and *n*-type. A spin fluctuation mechanism of pairing is probably the best candidate for describing HTSC in copper oxides [1, 2]. One of the unsolved problems is the underlying electronic structure and how the specific electronic properties of a given material provide the rich variety of different properties in cuprates of the *p*- and *n*-type, ruthenates, and layered $RuSr_2GdCu_2O_8$. We discuss this problem in the framework of the multiband *p–d* model of transition metal oxides.

FORMULATION OF THE PROBLEM

The necessary ingredient for discussing possible mechanisms of HTSC is the band structure of the fermionlike quasiparticles. However, it is a difficult subject for *ab initio* calculations due to the strong electron correlations. For this reason, we use a model approach which is based on the possibility of rewriting the exact full Hamiltonian of the system in terms of larger-scale variables. Described briefly, the essence of the approach is as follows. Suppose we have a set of Wannier functions belonging to a chosen elementary cell which is generated by some single-electron problem for the crystal symmetry of interest. Then, the full electron field operator can be written in the form of an expansion:

$$\psi_\sigma(r) = \sum_{jL} \chi_{jL}(r) a_{jL}.$$

Here, the index $j \equiv R_j$ gives the coordinate of the chosen elementary cell of the lattice, L is the composite index $L = \{\lambda, \sigma\}$, λ labels bands, and σ stands for the spin projection. Due to the orthogonality of the Wannier functions, we have $\{a_{jL}, a^+_{j'L'}\} = \delta_{jL,j'L'}$. The full nonrelativistic Hamiltonian can be written in the form of a sum of intra- (H_c) and intercell (H_{cc}) terms:

$$H = H_c + H_{cc} = \sum_i H_i^c + \sum_{i \neq j} H_{ij}^{cc},$$

$$H_i^c = \sum_{LL'} h_i^{LL'} a^+_{iL} a_{iL'} + \frac{1}{2}\sum_{LL'} v_{iL,iL',iL'',iL'''} a^+_{iL} a^+_{iL'} a_{iL''} a_{iL'''},$$

$$H_{ij}^{cc} = \sum_{LL'} h_{ij}^{LL'} a^+_{iL} a_{jL'}$$

$$+ \frac{1}{2}\sum_{LL'} v_{iL,jL',jL'',jL'''} a^+_{iL} a^+_{jL'} a_{jL''} a_{iL'''}$$

$$- \frac{1}{2}\sum_{LL'} v_{iL,jL',iL'',jL'''} a^+_{iL} a^+_{jL'} a_{iL''} a_{jL'''}.$$

Now suppose that we are able to find the many-electron states for the intracell Hamiltonian in an approximation better than Hartree–Fock, so that it takes into account (at least, partly) strong intra-atomic and intercluster interactions. Then,

$$H_i^c |i, \Gamma_n\rangle = E_{n\Gamma}^{(0)} |i, \Gamma_n\rangle$$

and the full Hamiltonian can be rewritten in terms of the Hubbard's operators

$$X_i^m \equiv X_i^{\Gamma_{n-1},\Gamma_n} \equiv |i, \Gamma_{n-1}\rangle\langle i, \Gamma_n|,$$

$$Z_i^\xi \equiv Z_i^{\Gamma_n,\Gamma_n'} \equiv |i, \Gamma_n\rangle\langle i, \Gamma_n'|.$$

The Hubbard model is often used to study the electronic structure of strongly correlated electron systems (SCES). To take into account the chemistry of metal oxides, it is generalized to the p–d model; the simplest version of such a model has been proposed by Emery [3] and Varma *et al.* [4]. In this 3-band p–d model, only the $d_{x^2-y^2}$ Cu and p_σ O orbitals are considered. There are many indications of the importance of the d_{z^2} Cu orbital (see review [5]). A multiband p–d model with both $d_{x^2-y^2}$ and d_{z^2} states has been proposed by Loktev *et al.* [6]. To calculate the electronic structure in SCES, the generalized tight-binding (GTB) method combining the exact diagonalization of the Hamiltonian for small clusters (intracell part of the Hamiltonian) with the cluster perturbation theory for the intercell part of the Hamiltonian was proposed by Ovchinnikov and Sandalov [7]. Recently, the electronic structure of the undoped antiferromagnetic (AF) insulator like $Sr_2CuO_2Cl_2$ and its evolution with doping have been studied by Gavrichkov *et al.* [8]. The dispersion equation in the GTB method for two sublattice AF states is given by

$$\left\| \frac{(E-\Omega_m^G)}{F_\sigma^G(m)}\delta_{mn} - 2\sum_{\lambda\lambda'}\gamma_{\lambda\sigma}^*(m)T_{\lambda\lambda'}^{PG}(\mathbf{k})\gamma_{\lambda'\sigma}(n)\right\| = 0, \quad (1)$$

where the zero frequency of the transition $\Omega_{i,m}^{(0)} = E_{n+1,\Gamma}^{(0)} - E_{n,\Gamma}^{(0)}$ is renormalized by the Coulomb interaction within the analogue of the Hubbard-I approximation as follows:

$$\delta_{mm_1}\Omega_{i,m} = \delta_{mm_1}\Omega_{i,m}^{(0)} + \sum_{j(\neq i)}\left(B_{ij}^{\Gamma_1\Gamma_2,\Gamma_3\Gamma_4}\varepsilon_{m_1}^{m,[\Gamma_1,\Gamma_2]}\langle Z_j^{\Gamma_3,\Gamma_4}\rangle - B_{ji}^{\Gamma_1\Gamma_2,\Gamma_3\Gamma_4}\varepsilon_{m_1}^{m,[\Gamma_3,\Gamma_4]}\langle Z_j^{\Gamma_1,\Gamma_2}\rangle\right),$$

where the matrix elements $B_{ij}^{\Gamma_1\Gamma_2,\Gamma_3\Gamma_4}$ are

$$B_{ij}^{\Gamma_1\Gamma_2,\Gamma_3\Gamma_4} = \nu_{iL,jL',jL'',iL'''}[a_{iL}^+a_{iL'''}]^{\Gamma_1\Gamma_2}[a_{jL'}^+a_{jL''}]^{\Gamma_3\Gamma_4}.$$

Here, excitations $[\Gamma_1, \Gamma_2]$ and $[\Gamma_3, \Gamma_4]$ are Bose-like ones, and the splitting in fermionlike excitations originates, obviously, from the crystal-field splitting of the states Γ by Coulomb interaction with the neighboring clusters. Against a background of $\Omega_{i,m}^{(0)}$, which is of the order of Hubbard's U of the cluster, these effects are small. Below, we consider the antiferromagnetic state and the lattice index i runs over the sublattices P, G.

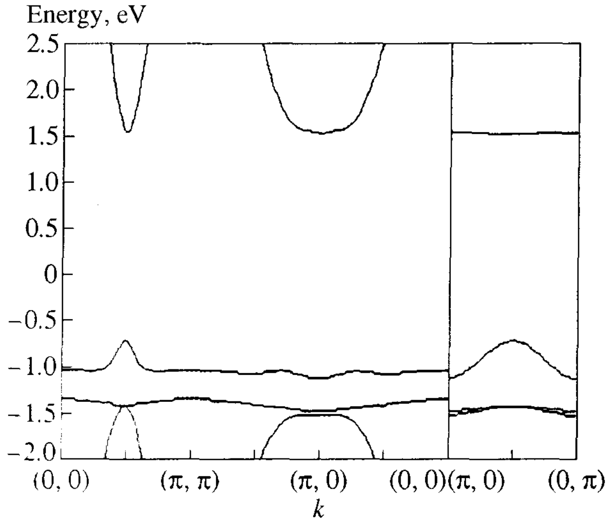

Fig. 1. Band structure of the undoped CuO_2 layer.

Here, $m \leftrightarrow (p, q)$ numerate a quasiparticle described by the Hubbard's operator X^{pq}, and $\gamma_{\lambda\sigma}(m)$ is a parameter of X-operator representation for the single-electron annihilation operator with orbital λ and spin σ,

$$a_{f\lambda\sigma} = \sum_m \gamma_{\lambda\sigma}(m)X_f^m.$$

Equation (1) has the same structure as the usual tight-binding equation of the single-electron approach but differs in the following: (i) the local energy Ω_m is given by the multielectron resonance $\Omega_m = E_{n+1}(p) - E_n(q)$, between the n- and $(n + 1)$-electron terms of the cell; (ii) filling factors $F(m) = \langle X^{pp}\rangle + \langle X^{qq}\rangle$ result in a concentration and temperature dependences of the band structure.

The electronic structure for the undoped case with hole concentration $n_h = 1$ is shown in Fig. 1. It was calculated for the following set of model parameters (in eV):

$$\begin{gathered} t_{pq} = 1, \quad \varepsilon(d_{x^2-y^2}) = 0, \quad \varepsilon(d_{z^2}) = 0, \\ \varepsilon(p_x) = 1.6, \quad \varepsilon(p_z) = 0.5, \\ t_{pp} = 0.46, \quad t'_{pp} = 0.4, \quad U_d = 9, \\ U_p = 4, \quad V_{pd} = 1.5, \quad J_d = 1. \end{gathered} \quad (2)$$

The wide charge transfer gap $E_{ct} \approx 2$ eV separates the empty conductivity band mainly of $d_{x^2-y^2}$ character and the filled valence band formed by a complex mixture of different copper and oxygen orbitals.

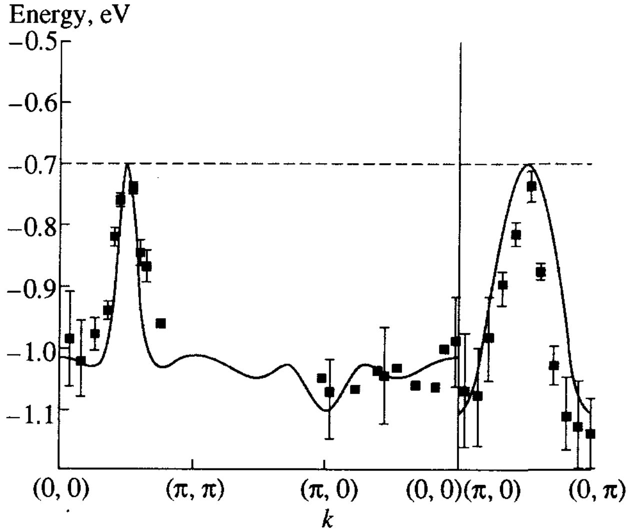

Fig. 2. The dispersion of the top part of the valence band in comparison with ARPES data on $Sr_2CuO_2Cl_2$ [9].

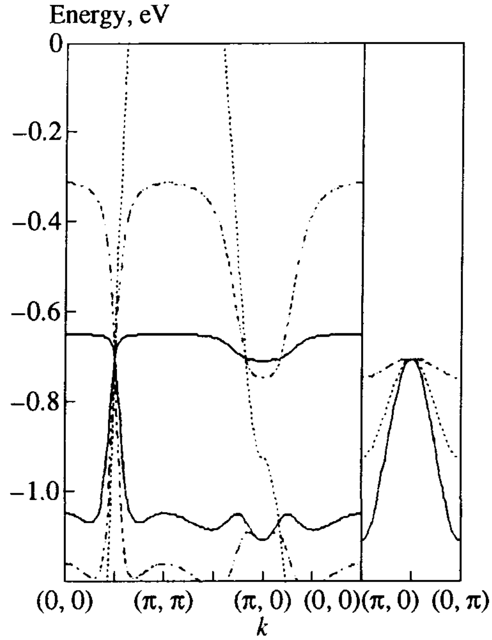

Fig. 3. Concentration dependence of the band structure in the antiferromagnetic (x = 0.01, solid line; x = 0.1, dot-dashed line) and paramagnetic (x = 0.2, dashed line) phases.

The dispersion of the top of the valence band is shown in Fig. 2 together with the ARPES data [9]. It should be noted that the valence band is formed by hole excitations from the initial single-hole state $|1, \sigma\rangle$ to different final two-hole states, both singlet $|S\rangle$ and triplet $|T, M\rangle$, $M = -1, 0, +1$ being essential. One more unusual result of GTB calculations [8] is the dispersionless virtual level shown by the dashed line in Fig. 2. It has zero weight in the undoped case but acquires the spectral weight $\sim x$ in the hole doped system with $n_h = 1 + x$, providing formation of the in-gap state at the top of the valence band. The dispersion of the in-gap state and its concentration evolution is shown in Fig. 3.

The calculation [8] was not self-consistent, magnetic order is given *ad hoc*. Thus, the curve for $x = 0.1$ in Fig. 3 is the interpolation, its justification being the large correlation length of the short-range antiferromagnetic order.

THE EFFECTIVE HAMILTONIAN OF THE SINGLET–TRIPLET *T–T'–J* MODEL

The t–t'–J model is derived by exclusion of the intersubband hopping between the low (LHB) and upper (UHB) Hubbard's subbands for the Hubbard model [10] and for the 3-band p–d model [11]. We write the Hamiltonian in the form

$$H = H_0 + H_1,$$

where the excitations via the charge transfer gap are included in H_1. Then, we define an operator $H(\varepsilon) = H_0 + \varepsilon H_1$ and make the unitary transformation

$$\tilde{H}(\varepsilon) = e^{-i\varepsilon\hat{S}}H(\varepsilon)e^{i\varepsilon\hat{S}}.$$

The vanishing of linear terms in ε of $\tilde{H}(\varepsilon)$ gives the equation for matrix $\hat{S}$:

$$H_1 + i[H_0, \hat{S}] = 0. \quad (3)$$

The effective Hamiltonian is obtained in the second order in ε and at $\varepsilon = 1$ is given by

$$\tilde{H} = H_0 + \frac{1}{2}i[H_1, \hat{S}]. \quad (4)$$

It is convenient to express the matrix $\hat{S}$ in terms of X-operators. Thus, for the multiband p–d model with a hole doping, the effective Hamiltonian has the form of a singlet–triplet t–t'–J model [12]:

$$\tilde{H} = H_0 + H_t + H_J, \quad (5)$$

where H_0 (unperturbed part of the Hamiltonian), H_t (kinetic part of $\tilde{H}$), and H_J (exchange part of $\tilde{H}$) are given by the following expressions:

$$H_0 = \sum_i\left(\varepsilon_1\sum_\sigma X_i^{\sigma\sigma} + \varepsilon_{2S}X_i^{SS} + \varepsilon_{2t}\sum_M X_i^{TMTM}\right)$$

$$H_t = \sum_{\langle i,j\rangle,\sigma} t_{ij}^{bb}X_i^{S\bar{\sigma}}X_j^{\bar{\sigma}S}$$

$$+ \sum_{\langle i,j\rangle,\sigma} t_{fg}^{aa}(\sigma\sqrt{2}X_i^{T0\bar{\sigma}} - X_i^{T2\sigma\sigma})(\sigma\sqrt{2}X_j^{\bar{\sigma}T0} - X_j^{\sigma T2\sigma})$$

$$+ \sum_{\langle i,j\rangle,\sigma} t_{ij}^{ab}2\sigma\gamma_b[X_i^{S\bar{\sigma}}(\sigma\sqrt{2}X_j^{\bar{\sigma}T0} - X_j^{\sigma T2\sigma}) + H.c.]$$

$$H_J = \frac{1}{2}\sum_{\langle i,j\rangle}(J_{ij}+\sigma J_{ij})\Big(\mathbf{S}_i\mathbf{S}_j - \frac{1}{4}n_in_j\Big)$$

$$-\frac{1}{2}\sum_{\langle i,j\rangle,\sigma}\delta J_{ij}X_i^{\sigma\sigma}X_j^{\sigma\sigma}.$$

The J_{ij} is the exchange integral $J_{ij} = 4\frac{(t_{ij}^{0b})^2}{E_{ct}}$, and δJ_{ij} is the correction to it (dependent on the triplet's contribution) $\delta J_{ij} = 2v^2\frac{(t_{ij}^{ab})^2}{E_{ct}}$. For the nearest neighbors ($i = 0, j = 1$), the estimation gives $\frac{\delta J_{iJ}}{J_{ij}} \sim 10^{-2}$.

Previously, the motion of triplet holes and the simplest version of the singlet–triplet model were studied in [13].

The problem may be treated within a regular diagram technique (DT) developed earlier for strongly correlated electron systems [14, 15]. Recently, a version of DT that allows the introduction of the exact expressions for self-energies and vertices via functional derivatives of the Green's functions and derives the perturbation expansion in terms of dressed Green's functions was derived [16]. Here, we can give only the idea of the DT, omitting the details. The effective Hamiltonian in terms of cluster variables can be written in the form

$$H = \sum_j E_{jm}^{(0)} + \sum_{jj',mm'} B_{jj'}^{\bar{a}a'}X_j^{\bar{a}}X_j^{a'}.$$

The commutation relations for these operators are $[X_j^a, X_{j'}^{\bar{a}'}] = \delta_{jj'}\varepsilon_b^{a\bar{a}'}Z_j^b$, where X_j^a are Fermi-like and Z_j^b are Bose-like operators; $[X_j^a, Z_{j'}^{\xi}] = \delta_{jj'}\varepsilon_b^{a\xi}X_j^b$. As shown in [16], the structure constants $\varepsilon_b^{a\bar{a}'}$, $\varepsilon_b^{a\xi}$ contain information on the overlapping of the many-electron states even in the case when they are constructed within the nonorthogonal basis set. The overlap matrices, however, will be replaced by the Kronecker symbols in the present model calculation. Introducing the Kadanoff-Baym S matrix [17], $S = \exp(-i\int d1\, U(1)Z(1))$ with external time-dependent field $U_{i_1}^{a_1}(t_1) \equiv U(1)$ (which causes the transitions a_1 between different states $|i_1, m\rangle$ of the same ion i_1) and, using equations of motion for $X(1)$, we obtain the closed system of equations for correlators $N(1) \equiv \langle TZ(1)\rangle_U = \langle TSZ(1)\rangle/\langle TS\rangle$ and Green's functions of quasi-fermion $G(1, 1') = -i\langle TX(1)X(1')\rangle_U$ and quasi-boson hoppings $K(1, 1') = -i(\langle TZ(1)Z(1')\rangle_U - \langle TZ(1)\rangle\langle TZ(1')\rangle_U)$ in terms of functional derivatives with respect to the following fields:

$$D_0^{-1}(1,2)G(2,1')$$
$$= P(1,1') + B(2,3)\varepsilon_4^{12}\Big(N(4) + i\frac{\delta}{\delta U(4)}\Big)G(3,1'),$$

where $D_0^{-1}(12) \equiv (\delta_{12}i\partial_{t_1} - A_{12}(t_1) - \Omega_{12}^0)\delta(t_1 - t_2)$, $A_{12}(t_1) \equiv \varepsilon_{3_b}^{1\bar{2}}U^{3_b}(t_1)$ and $P(1, 1') = \delta(t_1 - t_{1'})\varepsilon_{3_b}^{1\bar{2}}\langle Z^{3_b}(t_{1'})\rangle_U$.

We look for a solution in the form $G(3, 1') = D(3, 5)P(5, 1')$. Defining D by the equation $D^{-1}(1, 2) = D_0^{-1}(1, 2) - \Sigma(1, 2)$, the vertex as $\Gamma(1, 2; 3) = \delta D^{-1}(1, 2)/\delta U(3)$ and using the relation $\delta G(1, 2)/\delta U(3) = -D(1, 4)\Gamma(4, 5; 3)G(5, 2) + D(1, 4)\delta P(42)/\delta U(3)$ with $\delta P(42)/\delta U(3) = \varepsilon_6^{42}K(6, 3)$, we obtain a closed equation for the GF in terms of the vertices:

$$D_0^{-1}(1,2)G(2,1') = P(1,1') + \delta P(1,1')$$
$$+ B(2,3)\varepsilon_4^{12}N(4)G(3,1')$$
$$- B(2,3)\varepsilon_4^{12}D(36)\Gamma(6,7;4)G(7,1)$$

with $\delta P(1, 1') = B(2, 3)\varepsilon_4^{12}D(3, 5)\delta P(51)/\delta U(4)$. Iterating this exact equation via vertex and self-energy, we obtain an expansion in terms of dressed Green's functions.

For the electron-doped systems, the exclusion of all two-hole states results in the usual t–t'–J model. Thus, the asymmetry of the electronic structure of p- and n-type doped copper oxides results from the different structure of the Hilbert subspaces for $n_h = 0$ (one vacuum state $|0\rangle$) and $n_h = 2$ (a set of two-hole singlet $|S\rangle$ and triplet $|TM\rangle$, a Zhang-Rice singlet being one of them). In the low excitation energy region $E \ll \Delta$, where $\Delta = E_T - E_S$ is the energy of the lowest spin exciton, one can omit all excited two-hole states and obtain the effective t–t'–J model both for p- and n-type systems. The typical value of Δ is 0.5 eV. That is much less than the Mott-Hubbard or charge transfer gaps.

In the t–t'–J model, the difference between p- and n-type systems is provided by the different sign of the t'/t ratio. It was shown that to fit the ARPES data the following ratios are required [18]: for $La_{2-x}Sr_xCuO_4$ $t'/t = -0.2$, for $YBa_2Cu_3O_7$ $t'/t = -0.45$,and for $Nd_{2-x}Ce_xCuO_4$ $t'/t = +0.2$. A direct calculation [8] gives $t'_{\rm eff}/t_{\rm eff} = -0.24$ for the p-type doping.

MAGNETIC MECHANISM OF PAIRING FOR HOLE- AND ELECTRON-DOPED CUPRATES

An early suggestion that AF spin fluctuations could give rise to singlet $d_{x^2-y^2}$–wave pairing in hole-doped cuprate superconductors was made by Bickers, Scalapino, and Scalettar [19]. This suggestion has been supported by the FLEX approximation to the Hubbard model [20] that is, however, not valid in the case of $U \gg t$. In this limit of SCES, the proper model is the t–J model. Exact diagonalization and the quantum Monte Carlo method results for small clusters have been discussed by Dagotto [21]. For the infinite lattice, the most adequate perturbation approach to the t–J model has been formulated in the X-operator representation because of the exact treatment of local constraint due to X-operators algebra. The mean-field solution [22–24] of the t–J model and an analysis of the self-energy correlations beyond the mean-field approximation by the diagram technique [25] and by the high-order decoupling scheme [26] has confirmed the $d_{x^2-y^2}$-pairing in the hole-doped system with typical $T_c(x)$ dependence. Nevertheless, the optimal concentration of holes is $x_{opt} \approx 0.33$, which is twice more than the experimental value.

As concerns n-type cuprates, the gap symmetry was unclear for a long time. Recently, phase-sensitive tunnel experiments by Tsuei and Kirtley [27] found evidence for dominant $d_{x^2-y^2}$ symmetry in electron-doped cuprates. We obtain that the mean-field solution of the t–t'–J model results in $d_{x^2-y^2}$-gap symmetry for both p- and n-type systems. The difference in sign of t'/t provides a quantitative difference in the superconducting phase as well as in the normal phase.

COMPARISON OF MAGNETIC MECHANISMS OF PAIRING FOR CUPRATES AND RUTHENATES

The different electronic structure formed by $(t_{2g}-p)$–π bonding in ruthenates in comparison with $(d_{x^2-y^2}-p)$–σ bonding can result in a ferromagnetic coupling I between nearest Ru^{4+} ions. To compare superconductivity in cuprates and ruthenates, the t–J–I model has been proposed. Its mean-field solution [28, 29] has shown that, for $J \gg I$ (cuprates), there is the $d_{x^2-y^2}$ gap, while for $J \ll I$ (ruthenates) the triplet p symmetry gap occurs. The equation for T_c is similar in both cases, nevertheless the different gap symmetry results in a two orders of magnitude difference of T_c values. The reason is cancellation of the Van-Hove singularity for p-pairing, while for d-pairing high-T_c is a result of the spin-fluctuation mechanism in SCES enhanced by the Van-Hove singularity. A similar conclusion was obtained previously in [24, 30].

The coexistence of ferromagnetism and superconductivity in $RuSr_2GdCu_2O_8$ [31] can also be studied in the framework of the t–J–I model. Superconductivity in the CuO_2 layer ($J \gg I$) has $d_{x^2-y^2}$ symmetry, while for the RuO_2 layer ($J \ll I$) there is a competition of the ferromagnetic and triplet superconducting order. According to the mean-field phase diagram [32], a small decrease of hole concentration in the RuO_2 layer in comparison to Sr_2RuO_2 results in the magnetic phase.

CONCLUSION

A generalized tight-binding analysis of the realistic multiband p–d model gives rather good agreement with ARPES and other spectroscopic data for the whole range of doping and provides the effective low-energy Hamiltonian of the t–t'–J model. The mean-field solution of this model implies $d_{x^2-y^2}$ gap symmetry both for n- and p-type doped cuprates that is induced by AF spin fluctuations. In addition, the ferromagnetic fluctuation in the t–J–I model allows the comparison of magnetic pairing in cuprates and ruthenates on an equal footing.

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